## VII. CLAIMS

What is claimed is:

1. A method for treating Parkinson's disease, comprising administering to a subject a compound having the formula I

wherein

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A represents a cycloalkyl group, heterocycloalkyl group, an aryl group or heteroaryl group;

U is absent or when U is present, U represents -C(=O)-, -C(=S)-, -

10  $P(=O)(OR^5)$ -,  $-S(O_2)$ - or -S(O)-;

V is absent or when V is present, V is NR<sup>6</sup>, O or S;

Q is absent or when Q is present, V is NR<sup>6</sup>, O or S;

Y represents NR<sup>4</sup>, O or S;

X is, independently, C, N, S, Se or O;

R<sup>1</sup> is, independently, hydrogen, aryl, alkyl, alkoxy, hydroxy, hydroxyalkyl, aralkyl, halogen, cyano, aldehyde, ketone, ester, carbonate, amido, amino, alkylamino, nitro, thiol, thioalkyl or a sulfo-oxo group;

R<sup>2</sup> is hydrogen, aryl, alkyl, aralkyl, alkoxy, hydroxy, hydroxyalkyl, halogen, ester, carbonate, amido, amino, alkylamino, thiol or thioalkyl;

20 R<sup>3</sup> is, independently, hydrogen, aryl, alkyl, aralkyl, alkoxy, hydroxy, hydroxyalkyl, halogen, cyano, aldehyde, ketone, ester, carbonate, amido, amino, alkylamino, nitro or a sulfo-oxo group;

wherein the ring formed by X, Y and carbon b optionally contains a carbon-carbon double or carbon-oxygen double bond;

25 R<sup>4</sup> is hydrogen, alkyl, keto, aryl, aralkyl, heteroaryl or heteroaralkyl;

R<sup>5</sup>, R<sup>6</sup> and R<sup>7</sup> are, independently, hydrogen, alkyl, alkenyl, aryl, heteroaryl, aralkyl or heteroaralkyl;

m is an integer of from 0 or 1;

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n is an integer of from 0 to 7;

p is an integer of from 3 to 6;

q is an integer of from 0 to 16;

the stereochemistry at carbon a and carbon b is R or S;

or a pharmaceutically acceptable salt, pro-drug or metabolite thereof.

2. The method of Claim 1, wherein the compound has the formula II

wherein

U is absent or when U is present, U represents -C(=O)-, -C(=S)-, -

10  $P(=O)(OR^5)$ -,  $-S(O_2)$ - or -S(O)-;

V is absent or when V is present, V is NR<sup>6</sup>, O or S;

Q is absent or when Q is present, V is NR<sup>6</sup>, O or S;

R<sup>2</sup> is hydrogen, aryl, alkyl, aralkyl, alkoxy, hydroxy, hydroxyalkyl, halogen, ester, carbonate, amido, amino, alkylamino, thiol or thioalkyl;

R<sup>5</sup> and R<sup>6</sup> are, independently, hydrogen, alkyl, alkenyl, aryl, heteroaryl, aralkyl or heteroaralkyl;

s is an integer of from 0 to 2;

Ar is a substituted or unsubstituted aryl or heteroaryl group;

the stereochemistry at carbon a and carbon b is R or S;

or a pharmaceutically acceptable salt, pro-drug or metabolite thereof.

3. The method of Claim 1, wherein the compound has the formula III



wherein

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R<sup>8</sup> is hydrogen, aryl, alkyl, alkenyl, hydroxyalkyl, aralkyl, aldehyde, ketone, cycloalkyl, heteroaryl or the pharmaceutically acceptable salt thereof;

R<sup>9</sup> and R<sup>10</sup> are, independently, hydrogen, aryl, alkyl, alkenyl, alkoxy, hydroxy, hydroxyalkyl, aralkyl, halogen, cyano, aldehyde, ketone, ester, carbonate, amido, amino, alkylamino, thiol, thioalkyl, nitro or a sulfo-oxo group;

Z is  $-CH_2$ - or -C(=O)-;

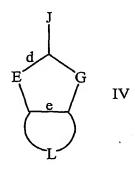
T is hydrogen or  $-C(=O)-N(R^{11})_2$ , wherein  $R^{11}$  is, independently, hydrogen, aryl, alkyl or aralkyl;

and the stereochemistry at carbon a and carbon b is R or S, or a pharmaceutically acceptable salt, pro-drug or metabolite thereof.

- 4. The method of Claim 3, wherein each R<sup>9</sup> is hydrogen and each R<sup>10</sup> is hydrogen.
- 15 5. The method of Claim 3, wherein Z is CH<sub>2</sub> and T is hydrogen.
  - 6. The method of Claim 3, wherein  $R^8$  is hydrogen or  $C_1$ - $C_8$  alkyl.
  - 7. The method of Claim 3, wherein  $R^8$  is methyl.
  - 8. The method of Claim 3, wherein the stereochemistry at carbons a and b is R.
  - 9. The method of Claim 3, wherein  $R^8$  is  $C_1$ - $C_8$  alkyl, each  $R^9$  is hydrogen, each
- 20 R<sup>10</sup> is hydrogen, Z is CH<sub>2</sub>, T is hydrogen, and the stereochemistry at carbons a and b is R.
  - 10. The method of Claim 3, wherein R<sup>8</sup> is methyl, each R<sup>9</sup> is hydrogen, each R<sup>10</sup> is hydrogen, Z is CH<sub>2</sub>, T is hydrogen, and the stereochemistry at carbons a and b is R.
  - 11. A method for treating Parkinson's disease, comprising administering to a subject d-threo methylphenidate.



12. A method for treating Parkinson's disease, comprising administering to a subject a compound having the formula IV



wherein

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when d is a single bond, E is S, O, C(R<sup>11</sup>)<sub>2</sub>, or NR<sup>11</sup>, and when d is double bond, E is CR<sup>11</sup> or N;

G is S, O, C(R<sup>11</sup>)<sub>2</sub>, or NR<sup>11</sup>;

J is hydrogen,  $C(R^{12})_3$ ,  $SR^{12}$ ,  $OR^{12}$ , or  $N(R^{12})_2$ ;

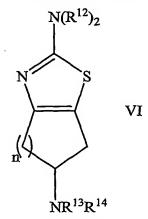
wherein R<sup>11</sup> and R<sup>12</sup> are, independently, hydrogen, aryl, alkyl, aralkyl, alkoxy, hydroxy, hydroxyalkyl, halogen, ester, carbonate, amido, amino, alkylamino, thiol or thioalkyl;

L is a fused substituted or unsubstituted cycloalkyl group, heterocycloalkyl group, aryl group, or heteroaryl group;

d is a single bond or a double bond; and

- e is a single bond or a double bond.
- 13. The method of claim 12, wherein d is a double bond and E is N.
- 14. The method of claims 12 and 13, wherein G is S.
- 15. The method of claims 12-14, wherein L is a cycloalkyl group.
- 16. The method of claim 15, wherein the cycloalkyl group is a cyclohexyl group
- 20 having at least one substituted or unsubstituted amino group.
  - 17. The method of claim 16, wherein the amino group is NHPr.
  - 18. The method of claims 12-17, wherein J is  $N(R^{12})_2$ .
  - 19. The method of claim 18, wherein each R<sup>12</sup> is hydrogen.
  - 20. The method of claims 12-19, wherein d and e are double bonds.
- 25 21. The method of claim 12, wherein the compound has the formula V

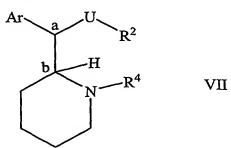
22. The method of claim 12, wherein the compound has the formula VI



wherein  $R^{13}$  and  $R^{14}$  are hydrogen, aryl, alkyl, aralkyl, hydroxyalkyl, or  $R^{13}$  and  $R^{14}$  form a cycloalkyl group or heterocycloalkyl group, and

n is from 0 to 3.

23. A method for treating Parkinson's disease, comprising administering to a subject a compound having the formula VII



10 wherein

U is -C(=O)-, -S(O<sub>2</sub>)- or -S(O)-;

R<sup>2</sup> is hydrogen, aryl, aralkyl;

R<sup>4</sup> is hydrogen, alkyl, keto, aryl, aralkyl, heteroaryl or heteroaralkyl; and the stereochemistry at carbon a and carbon b is R or S.



24. A method for treating Parkinson's disease, comprising administering to a subject a compound having the formula VIII

$$(H_2C)_n \xrightarrow{X} (C)_{\overline{y}} \xrightarrow{Z} R^1$$

$$(H_2C)_n \xrightarrow{X} (C)_{\overline{y}} \xrightarrow{Z} R^1$$

$$(R^8) \times R^8$$

$$(CR^5R^6)_m \times R^8$$

$$(R^8) \times R^8$$

## 5 wherein

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X represents  $C(R^3)_2$ , O, S, SO, SO<sub>2</sub>,  $NR^2$ ,  $NC(O)R^7$ ,  $NC(O)OR^2$ ,  $NS(O)_2R^7$ , or C=O;

Z represents C(R<sup>3</sup>)<sub>2</sub>, C(O), O, NR, NC(O)OR, S, SO, or SO<sub>2</sub>;

m is 1, 2, 3, 4 or 5;

10 n is 1 or 2;

p is 0, 1, 2, or 3;

y is 0, 1, or 2;

R<sup>1</sup> represents H, alkyl, cycloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl;

R1 represents H, alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl;

R and R<sup>1</sup> may be connected through a covalent bond;

R<sup>2</sup> represents independently for each occurrence H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl;

 $R^3$  represents independently for each occurrence H, alkyl, aryl,  $OR^2$ ,  $OC(O)R^2$ ,  $CH_2OR^2$ , or  $CO_2R^2$ ; wherein any two instances of  $R^3$  may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4 carbon atoms;

R<sup>4</sup> represents independently for each occurrence H, alkyl, cycloalkyl, aryl, heteroaryl, alkenyl, or OR;

R<sup>5</sup> and R<sup>6</sup> are selected independently for each occurrence from the group consisting of H, alkyl, (CH<sub>2</sub>)<sub>p</sub>Y, aryl, heteroaryl, F, OR<sup>2</sup>, and OC(O)R<sup>2</sup>; or an instance of CR<sup>5</sup>R<sup>6</sup> taken together is C(O);

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R<sup>7</sup> represents alkyl, cycloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; R<sup>8</sup> and R<sup>9</sup> are selected independently for each occurrence from the group consisting of H, alkyl, (CH<sub>2</sub>)<sub>p</sub>Y, aryl, heteroaryl, F, OR<sup>2</sup>, and OC(O)R<sup>2</sup>; or an instance of CR<sup>8</sup>R<sup>9</sup> taken together is C(O);

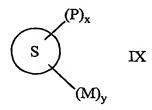
Y represents independently for each occurrence  $OR^2$ ,  $N(R^2)_2$ ,  $SR_2$ ,  $S(O)R^2$ ,  $S(O)_2R^2$ , or  $P(O)(OR^2)_2$ ; any two instances of  $R^2$  may be connected through a covalent bond;

a covalent bond may connect R<sup>4</sup> and an instance of R<sup>5</sup> or R<sup>6</sup>; any two instances of R<sup>5</sup> and R<sup>6</sup> may be connected through a covalent bond;

any two geminal or vicinal instances of R<sup>8</sup> and R<sup>9</sup> may be connected through a covalent bond;

and the stereochemical configuration at any stereocenter of a compound represented by A is R, S, or a mixture of these configurations.

25. A method for treating Parkinson's disease, comprising administering to a subject a A polypharmacophore having the formula IX:



wherein S comprises a scaffold unit; P comprises a pharmacophore unit, wherein x is greater than or equal to two; and M comprises a modifier unit, wherein y is greater than or equal to 0, whereby each one of P and M, for each occurrence, is appended to said scaffold unit, and whereby the polypharmacophore interacts with at least two biological targets.

- 26. A labeled compound comprising any one of compounds in claims 1-25.
- 27. A method for treating anxiety, autism, depression, sexual dysfunction, hypertension, migraine, Alzheimer's disease, obesity, emesis, psychosis, analgesia, schizophrenia, Parkinson's disease, Huntington's disease, restless leg syndrome, sleeping disorders, attention deficit hyperactivity disorder, irritable bowel syndrome, premature ejaculation, menstrual dysphoria syndrome, urinary incontinence, inflammatory pain, neuropathic pain, Lesche-Nyhane disease, Wilson's disease, or



Tourette's syndrome comprising administering to a subject a compound recited in claims 1-26.